Mathematical theory of defects

Part I. Statics

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The basic formulations of the theory of defects in the infinite, linearly elastic continuum are discussed. The point of departure is the displacement description and the theory of surface defects, which are represented by the elastic potentials of a double layer. The corresponding to it total distortion field splits up into its regular part, called elastic and singular part, called plastic or initial. The elastic stress field satisfies the equilibrium equation $\sigma_{ik,k} = 0$, which is the point of departure for the theory of initial deformations. Next we discuss the theory of dislocations, formulated with the help of elastic distortion field and the theory of disclinations formulated with the help of elastic strain and elastic bend-twist tensor. The transition to the general incompatibility problem is demonstrated together with the solution for an arbitrary anisotropy of the medium.

Omówione są podstawowe sformułowania teorii defektów w nieskończonym kontinuum liniowo sprężystym. Punktem wyjścia jest opis przemieszczeniowy i teoria defektów powierzchniowych, które są opisywane przez sprężyste potencjały warstwy podwójnej. Odpowiadające im całkowite pole dystorsji rozbija się na część regularną zwaną sprężystą i część osobliwą, zwaną plastyczną lub wstępną. Sprężyste pole naprężeń defektu powierzchniowego spełnia równanie równowagi $\sigma_{ik,k} = 0$, które jest punktem wyjścia dla teorii deformacji wstępnych. Następnie omówiona jest teoria dyslokacji sformułowana przy użyciu pola dystorsji sprężystej i teoria dysklinacji sformułowana przy użyciu tensora odkształcenia sprężystego i tensora giętno-skrętnego. Pokazane jest przejście do ogólnego problemu niezgodności i jego formalne rozwiązanie dla dowolnej anizotropii.

Обсуждены основные формулировки теории дефектов в бесконечном линейно упругом континуум. Исходной точкой являются описание в перемещениях и теория поверхностных дефектов, которые описываются упругими потенциалами двойного слоя. Отвечающие им полное поле дисторсий разбивается на регулярную часть, называемую упругой, и особую часть, называемую пластической или вступительной. Упругое поле напряжений поверхностного дефекта удовлетворяет уравнению равновесия $\sigma_{ik,k}=0$, которое является исходной точкой для теории начальных деформаций. Затем обсуждена теория дислокаций, сформулированная при использовании поля упругой дисторсии и теория дисклинаций, сформулированная при использовании тензора упругой деформации и изгибно-кручащего тензора. Показан переход к общей задачи несовместности и ее формальное решение для произвольной анизотропии.

1. Introduction

THE AIM of this work is to demonstrate relations between different formulations of the theory of defects. We shall consider defects in the linearly elastic, homogeneous, infinite medium. We shall discuss in principle those formulations of the theory which are applicable to the theory of dislocations and disclinations. Special methods of the two-dimensional crack theory will be omitted. We shall apply generalized functions technique.

In every formulation, the theory breaks up into geometrical conditions, which are at the same time the constraints equations and the methods of solution of the equilibrium equations, which result from the theory of elasticity.

From the classical theory of elasticity comes the diplacement description, to which corresponds the idea of an ideal medium. It is convenient to think of defects as of some forced deformations of the ideal medium. Deformations corresponding to defects are characterized by the fact that the displacement field u suffers discontinuities on certain surfaces inside the medium, called the defects surfaces. The discontinuous u field we treat further as a generalized function. The total distortion field $\mathbf{u}_{i,k}$, which corresponds to a defect in the displacement description, breaks up into its regular part 3 and singular part β , the latter having the character of a delta function concentrated on the defects surface. In the same way the total strain $\mathbf{u}_{\langle i,k\rangle}$ breaks up into its regular part \mathbf{e} and singular part e. The regular part of strain, and the stress field corresponding to it, always have a good physical interpretation; this is the elastic field corresponding to a defect. The singular part of strain has an interpretation of initial strain, in the theory of defects we call it plastic strain. The regular part of distortion field β , called the elastic distortion, has a good physical interpretation in the case of dislocations. This suggests the description applied in the theory of dislocations. We consider not the ideal medium described by means of the displacement field u with discontinuities, but the non-ideal medium described by the field of elastic distortions β . The field β satisfies the constraints equation, which formally is a relation between the derivatives of the elastic distortion β and plastic distortion $\dot{\beta}$; de facto, it is the field equation which describes the influence of the dislocations on the field β . The dislocations distribution is represented by the dislocation density tensor α .

A slightly different description is to be applied for the medium with disclinations. If the disclinations are present in the medium, no uniquely defined elastic distortion field exists; the state of elastic deformation is represented by means of elastic strain and what is called the elastic bend-twist tensor, which describes the relative rotation of the elements of the medium. In the constraints equations, the dislocation density tensor and the disclination density tensor appear.

As already indicated, for a defect of any kind the elastic strain field and elastic stress corresponding to it are well defined. For the ideal medium, the strain field satisfies the de Saint Venant compatibility equation. For the medium with defects, to which correspond plastic strains $\mathring{\mathbf{e}}$, the compatibility equation is not satisfied; instead, we have the constraints equations between what are called the incompatibilities of the fields \mathbf{e} and $\mathring{\mathbf{e}}$. We can thus describe the medium by means of elastic field \mathbf{e} to which the incompatibility tensor η corresponds. η is connected with the presence of defects in the medium; formally it is connected with the presence of plastic strains $\mathring{\mathbf{e}}$. This approach was formulated by E. Kröner.

2. The displacement description

2.1. Geometry

It is convenient to consider defects as certain forced deformations of the ideal elastic medium. We thus imagine that a defect was introduced into the medium by making a cut along some surface S and forcing some finite relative displacement U of the two faces of

the cut. Thus we define a surface defect as a surface of discontinuity of the displacement field **u**. Such a formulation has a clear geometric interpretation. If we use the displacement description, any defect is a surface defect. A point defect is a limiting case of a defect having the close surface converging to a point.

The displacement field **u** does not describe the state of the medium. We say that it is not the state quantity such as the stress and strain fields. Thus it may occur that in some cases it is not uniquely defined. For what are called linear defects, dislocations and disclinations, the elastic strain field produced in the medium by the defect, depends only on the defect line, which is the boundary of the surface S. Such defects are the whole class of the **u** fields having discontinuities on different surfaces with the same boundary.

In what follows, it will be convenient to assume that the function U admits the extension outside the surface S and can be represented as the function of the surface point ξ . The condition of discontinuity of the u field we write in the form:

$$(2.1) |[\mathbf{u}(\boldsymbol{\xi})]| = \mathbf{U}(\boldsymbol{\xi}); \quad \boldsymbol{\xi} \in S.$$

The double bracket denotes here the discontinuity of a function at the point ξ belonging to S. The condition (2.1), which we call here the geometric condition, is de facto the degenerate boundary condition.

Once U is given, the discontinuities of the tangent derivatives of the u field are prescribed. In what follows, we shall assume that U is an at least twice differentiable function of ξ . The derivatives of U with respect to ξ we denote by a comma:

$$(2.2) U_{i,k} \equiv \frac{\partial}{\partial \boldsymbol{\xi}_k} U_i.$$

Let us define the operator of tangent differentiation:

$$(2.3) D_k = \frac{\partial}{\partial \xi_k} - n_k n_s \frac{\partial}{\partial \xi_s},$$

where \mathbf{u} is the normal vector of the surface S. The geometric compatibility condition takes the form:

$$(2.4)_1 D_k U_i = |[u_{i,k}]| - n_k |[n_s u_{i,s}]|,$$

$$(2.4)_2 U_{i,k} - n_k n_s U_{i,s} = |[u_{i,k}]| - n_k n_s |[u_{i,s}]|.$$

2.2. Theory of elasticity

We have now to construct the displacement field corresponding to a defect in a linearly elastic, infinite medium.

The medium, when acted upon by a force density X(x), obeys the static Lamé equation(1):

$$(2.5) c_{iklm} \nabla_k \nabla_m u_l(\mathbf{x}) = -X_i(\mathbf{x}), \nabla_k = \frac{\partial}{\partial x_k},$$

⁽¹⁾ For the derivatives of the functions depending on x or $x-\zeta$ we shall apply both denotations: $f_{,k}$ and $\nabla_k f_{,k}$; they denote always the differentiation with respect to x_k , only for the functions of ζ , $f_{,k}$ denotes the differentiation with respect to ζ_k .

We accept force densities as being generalized functions. c is the tensor of elastic moduli of the medium. The particular solution of (2.5) has the form:

$$(2.6) u_i = G_{ik} \times X_k,$$

where G is the basic solution or the Green tensor of the Lamé equation:

$$c_{iklm}\nabla_k\nabla_mG_{jl}=-\delta_{ij}\delta_3(\mathbf{x}).$$

The star in (2.6) denotes the convolution with respect to the three spatial variables. For the isotropic medium:

$$(2.8)_1 c_{iklm} = \lambda \delta_{ik} \delta_{lm} + \mu (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}),$$

$$(2.8)_2 G_{ik}(\mathbf{x}) = \frac{1}{4\pi\mu} \left\{ \frac{\delta_{ik}}{r} - \frac{1}{2} \frac{\lambda + \mu}{\lambda + 2\mu} \nabla_i \nabla_k \cdot r \right\}, \quad r = |\mathbf{x}|,$$

 λ and μ are the Lamé constants.

Similarly as for the Laplace equation, for the static Lamé equation we have two important solutions called the elastic potential of a single and double layer. The theory of these potentials has been worked out by W. D. Kupradse [1], the applications to the defects theory having been elucidated by H. Zorski [2], see also the author's papers [3, 4, 5]. The role of the function $1/4\pi r$ is played by G, the role of the normal derivative by the operator

$$(2.9) \check{t}_{nr} = n_b c_{nbrs} \nabla_s,$$

 $t_{nr}u_r$ is the stress vector acting on the surface S. The potential of a double layer has the form:

$$(2.10) u_i = -\int_S ds_b U_n c_{nbrs} \nabla_s G_{ir}.$$

The above expression has the following properties:

$$(2.11)_1 \qquad |[u_i]| = \mathbf{U}_i,$$

$$(2.11)_2 |[\check{t}_{nr}u_r]| = 0.$$

We assume the potential of a double layer to describe a defect. The condition $(2.11)_2$ —the continuity of the stress vector on the defect's surface—ensures that a defect is a self-equilibrated formation.

Formally, we can write:

(2.12)
$$u_{i}G_{ir} \times \left[-\int_{S} ds_{b} U_{n} c_{nbrs} \nabla_{s} \delta_{3}(\mathbf{x}' - \boldsymbol{\xi}) \right]$$
$$= G_{ir} \times \left[-c_{nbrs} \nabla_{s} \int_{S} ds_{b} U_{n} \delta_{3}(\mathbf{x}' - \boldsymbol{\xi}) \right]; \quad \boldsymbol{\xi} \in S.$$

We can interpret the expressions in brackets as the force distribution producing the displacement field describing a defect. It is constructed of gradients of the delta function distributed over the surface S, and is thus a surface distribution of double forces. In view of the symmetry of the tensor c, it is the selfequilibrated distribution of forces, its resultant moment is equal to zero. The resultant force is also equal to zero. Consequently, in the

displacement description, the single static defect is equivalent to the selfequilibrated distribution of double forces X:

$$(2.13)_1 X_r = -\int_S ds g_{rs}(\xi) \nabla_s \delta_3(\mathbf{x} - \xi); \quad \xi \in S,$$

$$(2.13)_2 q_{rs} = c_{rsnb} U_n n_b.$$

This question was discussed in detail in [5].

Taking into account the condition (2.11)₂ and the geometric compatibility condition, we can calculate the normal derivative of the **u** field as a function of the derivatives of **U**. From the condition

(2.14)
$$0 = |[n_b c_{nbrs} u_{r,s}]| = n_b c_{nbrs} \{D_s U_r + n_s n_k |] [u_{r,k}]|\}$$
$$= n_b c_{nbrs} U_{\langle r,s \rangle} + c_{nbrs} n_b n_s \{-n_k U_{r,k} + n_k |[u_{r,k}]|\},$$

we calculate:

$$(2.15) -n_s U_{i,s} + n_s |[u_{i,s}]| = g_{ilm} U_{\langle l,m \rangle},$$

where the structure of the tensor g_{ilm} depends on the structure of c. Hence the discontinuity of the distortion field $u_{i,k}$:

$$|[u_{i,k}]| = U_{i,k} + n_k g_{ilm} U_{\langle l,m\rangle},$$

$$(2.16)_2 |[u_{\langle i,k\rangle}]| = [\delta_{il}\delta_{km} + n_{\langle k}g_{i\rangle lm}]U_{\langle l,m\rangle},$$

$$(2.16)_3 |[u_{i,k}]| = U_{i,k} + n_{i,k} g_{i,lm} U_{\langle l,m \rangle}.$$

The strain and stress fields are thus continuous through the surface if U is a constant vector or if $U_{\langle i,k\rangle} = 0$. These two cases realise the dislocations and disclinations. Disclinations are also called Volterra dislocations of the second kind (see [7, 8]). Dislocation is characterised by the constant Burgers vector **b**:

$$(2.17) U_i = -b_i, U_{i,k} = 0, |[u_{i,k}]| = 0,$$

disclination by the constant rotation vector Ω , and the position vector of the rotation axis $\dot{\xi}$:

(2.18)₁
$$U_i = -\varepsilon_{ipq} \Omega_p(\zeta_q - \mathring{\zeta}_q); \quad \xi \in S,$$

$$(2.18)_2 U_{i,k} = \varepsilon_{ikp} \Omega_p, |[\mathbf{u}_{\langle i,k\rangle}]| = 0, \quad |[u_{[i,k]}]| = \varepsilon_{ikp} \Omega_p.$$

By way of illustration, we derive now the important formula for the displacement field due to a dislocation; it will be represented as the sum of the discontinuous term, being the harmonic potential of a double layer, and the continuous term depending on the line only.

Let us introduce the Green potential K satisfying the Poisson equation (see [9]):

$$(2.19)_1 \Delta K_{ir} = -G_{ir},$$

$$(2.19)_2 K_{ir} = -\Delta^{-1}G_{ir} = G_{ir} \times \frac{1}{4\pi r}.$$

K also satisfies the equation:

$$(2.20) c_{iklm} \nabla_k \nabla_m K_{jl} = -\delta_{ij} \frac{1}{4\pi r}.$$

For the isotropic medium:

(2.21)
$$K_{ik} = \frac{1}{8\pi\mu} \left\{ -\delta_{ik} \cdot r + \frac{1}{12} \frac{\lambda + \mu}{\lambda + 2\mu} \nabla_i \nabla_k \cdot r^3 \right\}.$$

Then using (2.10), (2.17), $(2.19)_1$ we obtain:

$$(2.22) u_{i} = \int_{S} ds_{b} b_{n} c_{nbrs} \nabla_{s} G_{ir} = -\int_{S} ds_{b} b_{n} c_{nbrs} \nabla_{s} \nabla_{a} \nabla_{a} K_{ir}$$

$$= \int_{S} \left[ds_{b} \frac{\partial}{\partial \zeta_{a}} - ds_{a} \frac{\partial}{\partial \zeta_{b}} \right] b_{n} c_{nbrs} \nabla_{s} \nabla_{a} K_{ir} - \int_{S} ds_{a} b_{n} c_{nbrs} \nabla_{b} \nabla_{s} \nabla_{a} K_{ir}.$$

From (2.20) and the Stokes theorem:

(2.23)
$$\varepsilon_{alm} \int_{S} ds_{1} \frac{\partial}{\partial \zeta_{m}} f = \oint_{L} d\zeta_{a} f, \quad \int_{S} \left[ds_{k} \frac{\partial}{\partial \zeta_{b}} - ds_{b} \frac{\partial}{\partial \zeta_{k}} \right] f = \varepsilon_{kba} \int_{L} d\zeta_{a} f,$$

it follows then that (L is the boundary of S):

(2.24)
$$u_{i} = \oint_{L} d\zeta_{k} \varepsilon_{bak} b_{n} c_{nbrs} \nabla_{s} \nabla_{a} K_{ir} + \frac{b_{i}}{4\pi} \int_{S} ds_{a} \nabla_{a} \frac{1}{r}$$

The second discontinuous term does not give rise to the distortion discontinuity, since the derivatives of the harmonic potential of a double layer are continuous through the surface; this result is consistent with (2.17).

3. Elastic and plastic fields

3.1. Geometry

It can easily be proved (see (10)) that to a discontinuity U of the displacement field u on the surface S corresponds the singularity of the distortion field $\mathring{\beta}$, having the character of a delta function concentrated on the surface S. If we represent $u_{i,k}$ as (2)

$$(3.1) u_{i,k} = \beta_{ik} + \mathring{\beta}_{ik},$$

the singular term $\mathring{\beta}$ is equal:

(3.2)
$$\mathring{\beta}_{ik} = \int_{S} ds_k U_i \, \delta_3(\mathbf{x} - \mathbf{\xi}); \quad \mathbf{\xi} \in S.$$

 $\tilde{\beta}$ is called the initial or plastic distortion corresponding to a defect. The term *plastic* is rather in use in the defect theory. This term is motivated by the fact, that β represents that part of the deformation which is responsible for the discontinuity of the field u; in other words, it is the forced deformation which introduces a defect into the medium.

⁽²⁾ The denotations $u_{i,k} = \beta_{ki} + \mathring{\beta}_{ki}$ are in use in many publications.

The field β , which represents the deformation of the medium around the defect surface, is called the elastic distortion.

We introduce also the elastic and plastic strain field:

$$(3.3) u_{\langle i,k\rangle} = e_{ik} + \mathring{e}_{ik}.$$

The singular plastic surface distortion corresponding to a surface defect is of a more fundamental character than the plastic distortion corresponding to a point defect: $\mathring{\beta}_{lk} = \tau_{lk} \, \delta_3(\mathbf{x} - \mathbf{\zeta})$ (see [11]), the latter can be obtained from the former as a limit case; the form of a tensor τ will depend on the form of a point defect.

Note also that for line defects the plastic distortion $\mathring{\beta}$ is not uniquely defined. The surface S may be understood as a real surface, along which has occured the plastic slip giving rise to creation of defect, but it may also be some imaginary surface. It is not determined by the actual position of the line of the defect. The quantity $\mathring{\beta}$ may also be defined for the continuous distribution of defects, but even so it will not be determined uniquely by the distribution of defects.

Let us now discuss in detail the case of a dislocation. For a dislocation

(3.4)
$$\mathring{\boldsymbol{\beta}}_{ik} = -b_i \int_{S} ds_k \, \delta(\mathbf{x} - \boldsymbol{\xi}); \quad \boldsymbol{\xi} \in S,$$

b is the Burgers vector.

The notation

(3.5)
$$\int_{S} ds \, \delta_{3}(\mathbf{x} - \mathbf{\xi}) = \delta(S),$$
$$\int_{S} ds_{k} \, \delta_{3}(\mathbf{x} - \mathbf{\xi}) = n_{k}(\mathbf{\xi}) \, \delta(S),$$

is often in use; (see [12, 13]).

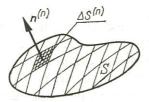


Fig. 1.

Note that the general expression (3.2) can be understood as a superposition of small dislocation loops $\Delta S^{(n)}$, each characterized by the Burgers vector $-\mathbf{U}^{(n)}(\text{Fig. 1})$:

(3.6)
$$\mathring{\beta}_{ik} = \int_{S} ds_{k} U_{i} \, \delta_{3}(\mathbf{x} - \mathbf{\xi}) = \sum_{n} U_{i}^{(n)} n_{k}^{(n)} \delta(\Delta S^{(n)}).$$

Such a formation is called a Somigliana dislocation. This idea is used when constructing what is called a dislocation model of a crack or a low angle grain boundary; we also speak of the dislocation model of a disclination.

From (3.1), we can eliminate the field **u** by acting with the rotation operator. We obtain the following relation:

$$\varepsilon_{klm} \nabla_l \beta_{im} = -\varepsilon_{klm} \nabla_l \mathring{\beta}_{im}.$$

We introduce the dislocation density tensor $\alpha(3)$: Lebest matrix which α products

$$\alpha_{ik} = -\varepsilon_{klm} \nabla_l \mathring{\beta}_{im}.$$

From the definition (3.8) follows that the divergence of α is equal to zero:

$$\alpha_{ik,k} = 0.$$

For a single dislocation line L:

(3.10)
$$\alpha_{ik} = -b_i \int_{S} ds_m \varepsilon_{klm} \frac{\partial}{\partial \zeta_l} \delta_3(\mathbf{x} - \mathbf{\xi}) = b_i \oint_{L} d\zeta_k \delta_3(\mathbf{x} - \mathbf{\xi}).$$

The components of the tensor α are proportional to the products of the appropriate components of the Burgers vector and the tangent vector of the dislocation line, moreover α is concentrated on the dislocation line; by contrast with $\mathring{\beta}$ it is determined by the actual position of the dislocation line. Thus α , not $\mathring{\beta}$ is a good source function of the theory and corresponds to the physical quantity-dislocation density. Note that, although (3.8) appears to be the definition of α in terms of $\mathring{\beta}$, it is α which is the primary quantity. $\mathring{\beta}$ should be so constructed that (3.8) may be satisfied. The tensor α admits generalisation to the case of continuous distribution of dislocations.

The Eq. (3.7) in the form

$$\varepsilon_{kim} \nabla_l \beta_{im} = \alpha_{ik}$$

may be understood as the constraints equation for the elastic distortion field β [14]. We can assume now, that β itself describes the non-ideal, or in the language of defect theory non-compatible medium in a state of elastic deformation. The incompatibility of the medium (in terms of β) describes the Eq. (3.11). Such a medium can be projected to an ideal medium only locally, in the areas where $\alpha=0$. This approach is close to physical reality.

The constraints equation for β , called also the Burgers condition, may be derived directly by examining the geometric properties of an elastic distortion field around a dislocation (see [3, 13]), without making use of the ideas of the u and β fields.

However when, in addition, disclinations are present in the medium, the incompatibilities are of more complicated nature and β is no longer a satisfactory physical quantity to describe the medium. (see [16, 17]). From (2.18)₂ it follows that the antisymmetric part of the distortion field is discontinuous on the disclination surface. We introduce the elastic and plastic rotation vectors:

$$(3.12)_{1} \qquad u_{i,k} = u_{\langle i,k \rangle} + u_{[i,k]}$$

$$= e_{ik} - \varepsilon_{ika} \omega_{a} + \mathring{e}_{ik} - \varepsilon_{ika} \mathring{\omega}_{a},$$

$$(3.12)_{2} \qquad |[\omega_{a}]| = -\Omega_{a}.$$

Since the discontinuity of the rotation vector $\boldsymbol{\omega}$ is constant over the surface S, its derivatives [by analogy with (3.1)] can be represented as the sum of the continuous part which we denote by $\boldsymbol{\varkappa}$ and the singular part $\boldsymbol{\phi}$:

$$\omega_{a,m} = \kappa_{am} + \mathring{\varphi}_{am}$$

⁽³⁾ The here defined α is the transpose of that used in [8, 15, 18, 19].

 κ is called by de Wit the elastic bend-twist tensor, $\mathring{\mathbf{\phi}}$ is called by Mura the plastic rotation field (see [8, 16])(4). The sum of $\mathring{\mathbf{\phi}}$ and $\mathring{\omega}_{a,m}$ will be denoted by $\mathring{\kappa}$ —the plastic bend-twist tensor:

$$\hat{\varkappa}_{am} = \mathring{\omega}_{a,m} + \mathring{\varphi}_{am} ;$$

then

$$(3.15)_1 u_{i,km} = e_{ik,m} - \varepsilon_{ika} \varkappa_{am} + \mathring{e}_{ik,m} - \varepsilon_{ika} \varkappa_{am},$$

$$(3.15)_2 u_{i,kml} = e_{ik,ml} - \varepsilon_{ika} \varkappa_{am,l} + \mathring{e}_{ik,ml} - \varepsilon_{ika} \varkappa_{am,l}.$$

For a single disclination, the plastic distortion by (3.2), (2.18)₂ is:

(3.16)
$$\mathring{\beta}_{ik} = -\oint_{S} ds_{k} \varepsilon_{ipq} \Omega_{p}(\zeta_{q} - \mathring{\zeta}_{q}) \, \delta_{3}(\mathbf{x} - \mathbf{\xi}),$$

the plastic rotation field, by analogy with (3.1), (3.2) is:

(3.17)
$$\mathring{\varphi}_{ik} = -\int_{S} ds_k \Omega_i \delta_3(\mathbf{x} - \mathbf{\xi}).$$

From $(3.15)_{1,2}$ follow the two constraints equations, being the relations between e, κ and e, κ :

$$(3.18)_1 u_{i,[km]} = 0,$$

$$(3.18)_2 \qquad \qquad \varepsilon_{klm}[e_{im,l} - \varepsilon_{ima} \varkappa_{al}] = -\varepsilon_{klm}[\mathring{e}_{im,l} - \varepsilon_{ima} \mathring{\varkappa}_{al}],$$

and

$$(3.19)_1 u_{i,k[ml]} = 0,$$

$$(3.19)_2 \qquad \qquad \varepsilon_{nlm} \varkappa_{am,l} = -\varepsilon_{nlm} \mathring{\varkappa}_{am,l}.$$

We define the two source quantities: the dislocation density tensor α and the disclination density tensor $\theta(5)$:

$$(3.20)_1 \qquad \qquad \alpha_{ik} = -\varepsilon_{klm} [\hat{e}_{im,l} - \varepsilon_{ima} \hat{\varkappa}_{al}],$$

$$(3.20)_2 \theta_{an} = -\varepsilon_{nlm} \mathring{\varkappa}_{am,l}.$$

In terms of $\mathring{\beta}$ and $\mathring{\phi}$, α and θ are:

$$\alpha_{ik} = -\varepsilon_{klm} [\mathring{\beta}_{im,l} - \varepsilon_{ima} \mathring{\varphi}_{al}],$$

$$\theta_{an} = -\varepsilon_{nlm}\mathring{\varphi}_{am,l}.$$

From the definitions $(3.20)_{1,2}$, the following compatibility equations for α and θ follow:

$$(3.22)_1 \alpha_{ik,k} - \varepsilon_{iam} \theta_{am} = 0,$$

$$(3.22)_2 \qquad \qquad \theta_{an,n} = 0.$$

For a single disclination line L, from (3.16), (3.17) we obtain:

$$(3.23)_1 \alpha_{ik} = \oint_L d\zeta_n \varepsilon_{ipq} \Omega_p(\zeta_q - \mathring{\zeta}_q) \, \delta_3(\mathbf{x} - \mathbf{\zeta}),$$

$$\theta_{an} = \oint_L d\zeta_n \Omega_a \, \delta_3(\mathbf{x} - \mathbf{\xi}).$$

⁽⁴⁾ The transposes of κ and φ are used in [8, 16].

⁽⁵⁾ The transposes of α and Θ are used in [8, 16].

Both densities α and θ are concentrated on the line only. α is proportional to the product $\Omega \times (\xi - \mathring{\xi})$; thus, when the disclination line ξ coincides with the rotation axis, α is equal to zero. The variation of ξ with respect to rotation axis is equivalent to the addition of a dislocation with the Burgers vector $\Omega \times (\xi - \mathring{\xi})$ to the disclination line. If both the dislocations and disclinations are simultaneously present in the medium then α defined by $(3.21)_1$, with $\mathring{\beta}$ understood as due to dislocations and disclinations, is the combined dislocation density tensor. When there are no plastic rotations in the medium, the definition $(3.21)_1$ coincides with (3.8).

3.2. Theory of elasticity

Notice first, that the elastic potential of a double layer (2.10) can by (2.12) and (3.4) be written as:

$$(3.24) u_i = G_{ir} \times [-c_{nbrs} \nabla_s \mathring{\beta}_{nb}] = -G_{ir} \times c_{nbrs} \nabla_s \mathring{e}_{nb}.$$

From the above it follows(6) that:

(3.25)
$$u_{i,k} = -G_{ir} + c_{nbrs} \nabla_s \nabla_k \mathring{\beta}_{nb} \pm G_{ir} c_{nbrs} \nabla_s \nabla_b \mathring{\beta}_{nk} =$$
$$= G_{ir} + c_{nbrs} \nabla_s [\mathring{\beta}_{nk,b} - \mathring{\beta}_{nb,k}] + \mathring{\beta}_{ik},$$

or in terms of e:

(3.26)
$$u_{i,k} = G_{ir} + c_{nbrs} \nabla_s [\mathring{e}_{nb,k} - \mathring{e}_{nk,b}] + \mathring{e}_{ik}.$$

To be in agreement with (3.1), we have to identify (7):

$$\beta_{ik} = G_{ir} + c_{nbrs} \nabla_s [\mathring{\beta}_{nk,b} - \mathring{\beta}_{nb,k}],$$

$$(3.27)_2 e_{ik} = G_{ir} + c_{nbrs} \nabla_s [\mathring{e}_{nn,b} - \mathring{e}_{nb,k}]_{\langle ik \rangle}.$$

We derive now the formula for β starting immediately from (2.10):

$$(3.28) u_{i,k} = -\int_{S} ds_{b} U_{n} c_{nbrs} \nabla_{s} \nabla_{k} G_{ir} \pm \int_{S} ds_{k} U_{n} c_{nbrs} \nabla_{s} \nabla_{b} G_{ir} =$$

$$= \int_{S} \left[ds_{b} \frac{\partial}{\partial \zeta_{k}} - ds_{k} \frac{\partial}{\partial \zeta_{b}} \right] U_{n} c_{nbrs} \nabla_{s} G_{ir}$$

$$- \int_{S} \left[ds_{b} U_{n,k} - ds_{k} U_{n,b} \right] c_{nbrs} \nabla_{s} G_{ir} + \int_{S} ds_{k} U_{i} \delta_{3} (\mathbf{x} - \mathbf{\xi})$$

$$= \oint_{I} d\zeta_{a} \varepsilon_{bka} U_{n} c_{nbrs} \nabla_{s} G_{ir} - \int_{S} \left[ds_{b} U_{n,k} - ds_{k} U_{n,b} \right] c_{nbrs} \nabla_{s} G_{ir} + \mathring{\beta}_{ik},$$

thus:

(3.29)
$$\beta_{ik} = \oint_L d\zeta_a \varepsilon_{bka} U_n c_{nbrs} \nabla_s G_{ir} - \int_S [ds_b U_{n,k} - ds_k U_{n,b}] c_{nbrs} \nabla_s G_{ir}.$$

The first term of the above expression is continuous on S, the second one is at least discontinuous on S and does not have the singularities of the delta function type.

⁶⁾ Here ± means the simultaneous addition and subtraction of a term.

⁷⁾ Here $\langle ik \rangle$ means the symmetrisation of the whole expression with respect to indices i, k.

We can generalize formulae (3.24), (3.25), (3.26) and (3.27)₁, ₂ to the arbitrary distribution of defects and the plastic distortion field corresponding to it.

The u field given by (3.24) is a solution of the equation:

$$(3.30) c_{iklm}u_{l,mk} = -c_{iklm}\nabla_m\nabla_kG_{lr} + c_{nbrs}\nabla_s\mathring{e}_{nb} = c_{isnb}\nabla_s\mathring{e}_{nb}.$$

From this it follows that the elastic field e satisfies the equation:

$$(3.31) c_{iklm} \nabla_k e_{lm} = 0.$$

The above important result can be obtained also by direct calculation:

$$(3.32) c_{iklm}c_{nbrs}\nabla_k\nabla_s\left[\int_{S}ds_mU_nG_{lr,b}-\int_{S}ds_bU_nG_{lr,m}\right]=$$

$$=c_{iklm}\nabla_k\int_{S}ds_mU_l\delta_3(\mathbf{x}-\mathbf{\xi})-\delta_{ir}c_{nbrs}\nabla_s\int_{S}ds_bU_n\delta_3(\mathbf{x}-\mathbf{\xi})=0.$$

By σ we indicate the elastic stress due to the elastic strain e:

$$\sigma_{ik} = c_{iklm}e_{lm},$$

Thus:

$$\sigma_{ik,k} = 0.$$

When solving the problem of stresses due to initial deformations, we always assume the Eq. (3.34) for the elastic stress due to initial deformation. Here we find some justification for this procedure, since for a surface defect, which is a fundamental form of initial deformation, the part of the stress which has the interpretation of elastic stress satisfies the Eq. (3.34) identically.

When we have to deal with an incompatible medium, which we describe by incompatible elastic fields, we take the Eq. (3.34) together with the constraints equations as the basic set of equations of the theory. Let us consider the medium with dislocations, which can be described in terms of elastic distortion field β . The set of equations

$$(3.35)_1 c_{iklm} \nabla_k e_{lm} = 0,$$

$$(3.35)_2 \qquad \qquad \varepsilon_{klm} \nabla_l \beta_{lm} = \alpha_{ik},$$

has to be simultaneously satisfied. Multiplying (3.35)₂ by ε_{abk} we obtain:

(3.36)
$$\beta_{ib,a} - \beta_{ia,b} = \varepsilon_{abk} \alpha_{ik} = -[\mathring{\beta}_{ib,a} - \mathring{\beta}_{ia,b}].$$

Now, we differentiate $(3.35)_1$:

$$(3.37) 0 = c_{iklm} \nabla_k \nabla_s e_{lm} \equiv c_{iklm} \nabla_k \nabla_s \beta_{lm}$$
$$\equiv c_{iklm} \nabla_k \nabla_m \beta_{ls} + c_{iklm} \nabla_k [\beta_{lm,s} - \beta_{ls,m}].$$

From (3.36), (3.37) follows the equation of the Lamé type for the field β :

$$(3.38) c_{iklm} \nabla_k \nabla_m \beta_{ls} = c_{iklm} \nabla_k \varepsilon_{msr} \alpha_{lr}.$$

The particular solution of (3.38) has the form:

$$\beta_{is} = G_{ij} + c_{jklm} \nabla_k \varepsilon_{smr} \alpha_{lr}$$

and is equivalent to:

(3.40)
$$\beta_{is} = G_{ij} + c_{jklm} \nabla_k [\beta_{ls,m} - \beta_{lm,s}],$$

which is in agreement with $(3.27)_1$.

We present here the formal solution of the Eq. (3.38) in terms of the Green function G. It is known that for most of the anisotropic bodies, G is not known in the closed form. However, for some cases of special geometry—for example the rectilinear screw dislocation perpendicular to the symmetry surface (see [21])— it is possible to find the solution of (3.38) in the closed form.

The set of equations:

(3.41)
$$\begin{cases} \langle u_{i,k} \rangle = e_{ik} + \mathring{e}_{ik} \\ \sigma_{ik,k} = 0 = c_{iklm} e_{lm,k} \end{cases} = u_i = G_{ir} \times c_{nbrs} \mathring{e}_{nb,s}$$

is also postulated in thermoelasticity. Initial strain $\mathring{\mathbf{e}}$ is given there as a function of the temperature. However, there is a difference in the interpretation of the quantities we deal with, since in thermoelasticity \mathbf{u} and $\mathbf{\sigma}$ are the real quantities, while \mathbf{e} and $\mathring{\mathbf{e}}$ are the subsidiary ones; whereas in the defect theory \mathbf{e} and $\mathbf{\sigma}$ are the real quantities, while \mathbf{u} and $\mathring{\mathbf{e}}$ are the subsidiary ones.

4. The incompatibility problem

4.1. Geometry

From $(3.27)_2$ we conclude that the elastic strain field e, and therefore also the elastic stress σ , can be represented in terms of $\mathring{\mathbf{e}}$ alone. Moreover, it is e which describes the state of the body and which appears in the equations of equilibrium. It is important thus to derive the constraints equations for the e field when the plastic $\mathring{\mathbf{e}}$ field is prescribed. When we have to deal with defects, the $\mathring{\mathbf{e}}$ field is given as the symmetric part of (3.2), but the formulae derived in this section are applicable to any problem with initial strains $\mathring{\mathbf{e}}$.

The following identity for the derivatives of the u field takes place:

(4.1)
$$u_{i,km} = \frac{1}{2} \left[u_{i,km} + u_{k,im} \right] + \frac{1}{2} \left[u_{i,mk} + u_{m,ik} \right] - \frac{1}{2} \left[u_{k,mi} + u_{m,ki} \right].$$

Inserting into the above formula the expression $u_{\langle i,k\rangle} = e_{ik} + \mathring{e}_{ik}$, we obtain:

$$u_{i,km} = e_{ik,m} + e_{im,k} - e_{km,i} + \mathring{e}_{ik,m} + \mathring{e}_{im,k} - \hat{e}_{km,i}$$

and

$$u_{i,kml} = e_{ik,ml} + e_{im,kl} - e_{km,il} + \mathring{e}_{ik,ml} + \mathring{e}_{im,kl} - \mathring{e}_{km,il}.$$

Simultaneously,

$$u_{i,klm} = e_{ik,lm} + e_{il,km} - e_{kl,im} + \hat{e}_{iklm} + \hat{e}_{il,km} - \hat{e}_{kl,im}.$$

Subtracting (4.4) from (4.3), we obtain:

$$(4.5) e_{im,kl} + e_{kl,im} - e_{km,il} - e_{il,km} = -\left[\hat{e}_{im,kl} + \hat{e}_{kl,im} - \hat{e}_{km,il} - \hat{e}_{il,km}\right].$$

In view of the antisymmetry in the indices (i, k), (l, m), we can write (4.5) in the form:

$$\varepsilon_{rik}\varepsilon_{plm}e_{km,il} = \varepsilon_{rik}\varepsilon_{plm}e_{km,il}.$$

This is the basic constraints equation for the effeld in the presence of initial (plastic) e field. When there are only elastic deformations in the medium, (e = 0), (4.5) is the classical de Saint Venant compatibility equation for the strain field. We define the incompatibility tensor η (the definition of η is due to Kröner [18]):

$$\eta_{ij} = \varepsilon_{ikl}\varepsilon_{jmn}\mathring{e}_{ln,km}.$$

The constraints equation (4.6) for the field e now takes the form:

$$\varepsilon_{rik}\,\varepsilon_{plm}e_{km,il}=\eta_{pr}.$$

From the definition (4.7) it follows that η is a symmetric tensor and that the divergence of η is equal to zero:

$$\eta_{ij,j} = \mathbf{0}_{\bullet}$$

Let us now explain the role of the incompatibility tensor.

Since a vector field can be represented as the sum of the gradient of a scalar field and the rotation of the vector field, a symmetric tensor can be represented as the sum of the symmetric part of a gradient of a vector field and the "double rotation" of a symmetric tensor field (see [18, 19]). We derive such a representation for the e field. We make use of the identity:

(4.10)
$$\Delta \Delta \frac{r}{8\pi} \simeq -\delta_3(\mathbf{x}).$$

We have thus:

$$(4.11) \quad \hat{e}_{ik} \equiv \hat{e}_{ik} \times \delta_{3}(\mathbf{x}) = -\hat{e}_{ik} \times \Delta \Delta \frac{r}{8\pi} = -\hat{e}_{ik,aabb} \times \frac{r}{8\pi}$$

$$= -\frac{r}{8\pi} \times \left\{ \nabla_{a} \nabla_{b} \left[\hat{e}_{ik,ab} + \hat{e}_{ab,ik} - \hat{e}_{ak,ib} - \hat{e}_{ib,ak} \right] - \nabla_{a} \nabla_{b} \left[\hat{e}_{ab,ik} - \hat{e}_{ak,ib} - \hat{e}_{ib,ak} \right] \right\} =$$

$$= -\frac{r}{8\pi} \times \left\{ \nabla_{a} \nabla_{b} \varepsilon_{iac} \varepsilon_{cde} \left[\hat{e}_{dk,eb} - \hat{e}_{db,ek} \right] - \nabla_{i} \nabla_{k} \hat{e}_{ab,ab} + \nabla_{i} \hat{e}_{ak,abb} + \nabla_{k} \hat{e}_{ib,baa} \right\} =$$

$$= -\frac{r}{8\pi} \times \left\{ \varepsilon_{iac} \varepsilon_{kbg} \nabla_{a} \nabla_{b} \varepsilon_{ced} \varepsilon_{gnj} \nabla_{e} \nabla_{n} \hat{e}_{dj} + \nabla_{i} \left[e_{ka,abb} - \frac{1}{2} \hat{e}_{ab,abk} \right] + \nabla_{k} \left[\hat{e}_{ia,abb} - \frac{1}{2} \hat{e}_{ab,abi} \right] \right\}.$$

If we define

$$\varphi_i = [\mathring{e}_{ab,abi} - 2\mathring{e}_{ia,abb}],$$

$$\Phi_{i} = \frac{r}{8\pi} \times \left[\hat{e}_{ab,abi} - 2\hat{e}_{ia,abb}\right]$$

and take into account the definition (4.7), (4.11) takes the form:

(4.13)
$$\hat{e}_{ik} = \Phi_{\langle i,k \rangle} - \varepsilon_{iab} \varepsilon_{kcd} \nabla_a \nabla_c \eta_{bd} \times \frac{r}{8\pi}.$$

The term $\Phi_{\langle i,k\rangle}$ can be considered as due to the displacement field Φ , the second term describing the incompatibility of the field $\hat{\mathbf{e}}$. As will be seen, only the incompatibility of the initial strain $\hat{\mathbf{e}}$ gives rise to the elastic strain \mathbf{e} .

Let us now calculate η in terms of dislocation density α and disclination density θ . Taking into account (4.7) and (3.20)₁, ₂, we obtain (see (16)):

(4.14)
$$\eta_{ij} = \varepsilon_{ikl}\varepsilon_{jmn}\nabla_{k}\nabla_{m}\mathring{e}_{ln} \\
= \varepsilon_{ikl}\varepsilon_{jmn}\nabla_{k}[\mathring{e}_{ln,m}\pm e_{lna}\mathring{x}_{am}] \\
= -\varepsilon_{ikl}\nabla_{k}\alpha_{lj} + \varepsilon_{ikl}\nabla_{k}[\mathring{x}_{jl} - \delta_{jl}\mathring{x}_{aa}] \\
= -\varepsilon_{ikl}\alpha_{lj,k} - \theta_{ji} + \varepsilon_{ijk}\nabla_{k}\mathring{x}_{aa}, \\
\eta_{ij} = -[\varepsilon_{ikl}\alpha_{lj,k} + \theta_{ji}]_{\langle ij \rangle}.$$

For a single disclination line, η is concentrated at the line only. Where there are only disclinations present in the medium,

$$\eta_{ij} = -\varepsilon_{ikl}\alpha_{lj,k\langle ij\rangle}.$$

4.2. The elastic strain field

The incompatibility problem for the elastic medium is thus formulated as follows. The medium with incompatibilities satisfies the following set of equations:

(4.17)₁
$$\sigma_{ij,j} = 0,$$
(4.17)
$$\varepsilon_{ikl}\varepsilon_{jmn}e_{ln,km} = \eta_{ij}.$$

The first is the equilibrium equation, the second is the constraints equation. The method of solution of the set of equations $(4.17)_1$, $(4.17)_2$ was presented in [9]. Here we shall find the elastic strain due to incompatibilities by making use of the formula $(3.27)_2$, where e is given in terms of \mathring{e} :

$$(4.18) e_{is} = G_{ij} \times c_{jklm} \nabla_k [\mathring{e}_{ls,m} - \mathring{e}_{lm,s}]_{\langle is \rangle}.$$

From (4.13) it follows that:

$$(4.19) \quad \mathring{e}_{ls,m} - \mathring{e}_{lm,s} = \varepsilon_{smp} \varepsilon_{pgr} \mathring{e}_{lg,r} = \left\{ \frac{1}{2} \left[\varphi_{l,sm} + \varphi_{s,lm} - \varphi_{l,ms} - \varphi_{m,ls} \right] \right. \\ \left. - \varepsilon_{smp} \varepsilon_{pgr} \varepsilon_{lab} \varepsilon_{gcd} \nabla_{a} \nabla_{c} \nabla_{r} \eta_{bd} \right\} \times \frac{r}{8\pi} = \left\{ \frac{1}{2} \left[\varphi_{s,ml} - \varphi_{m,sl} \right] \right. \\ \left. - \varepsilon_{smp} \varepsilon_{lab} \nabla_{a} \left[\nabla_{c} \nabla_{c} \eta_{bp} - \nabla_{p} \nabla_{r} \eta_{br} \right] \right\} \times \frac{r}{8\pi} .$$

The divergence of η is equal to zero, $\Delta r = \frac{2}{r}$, we thus obtain:

$$(4.20) \qquad \qquad \mathring{e}_{ls,m} - \mathring{e}_{lm,s} = \Phi_{[s,m]l} + \varepsilon_{smp} \varepsilon_{alb} \nabla_a \eta_{bp} + \frac{1}{4\pi r}.$$

We insert (4.20) into (4.18):

$$(4.21) e_{is} = G_{ij} + c_{jklm} \nabla_k \nabla_l \Phi_{[s,m]} + G_{ij} + \frac{1}{4\pi r} + c_{jklm} \nabla_k \varepsilon_{smp} \varepsilon_{alb} \nabla_a \eta_{bp}.$$

We make use now of (2.8) and the definition of the K tensor (2.19)2:

$$(4.22) e_{is} = \Phi_{[i,s]} + K_{ij} + C_{jklm} \nabla_k \nabla_a \varepsilon_{smp} \varepsilon_{alb} \eta_{bp \langle is \rangle}.$$

The asymmetric term $\Phi_{[i,s]}$ does not contribute, thus

$$(4.23) e_{is} = K_{ij} + c_{jklm} \nabla_k \nabla_a \varepsilon_{smp} \varepsilon_{alb} \eta_{bp\langle is \rangle}.$$

It is evident from the above formula, that in the static case only the incompatibility of the initial strain gives rise to the elastic strain e. However, to reconstruct \mathbf{u} we need to know \mathbf{e} and \mathbf{e} , not only \mathbf{e} and $\boldsymbol{\eta}$.

We define the incompatibility source tensor I (introduced by SIMMONS and BULLOUGH [20]):

$$I_{isbp} = \varepsilon_{smp} \varepsilon_{alb} c_{jklm} \nabla_k \nabla_a K_{ij\langle is \rangle}.$$

Then

$$(4.25 e_{is} = I_{isbp} + \eta_{bp}.$$

For the isotropic medium, the I tensor can easily be calculated and is equal:

$$(4.26) I_{isbp} = \left\{ -\delta_{sb}\delta_{ip}\Delta + \delta_{is}\delta_{bp}\Delta - \frac{2(\lambda+\mu)}{\lambda+2\mu}\delta_{bp}\nabla_{i}\nabla_{s} \right\} \cdot \frac{r}{8\pi}.$$

Therefore,

$$(4.27) e_{is} = \frac{r}{8\pi} \times \left\{ -\eta_{is,kk} + \eta_{kk,rr} \delta_{is} - \frac{2(\lambda + \mu)}{\lambda + 2\mu} \eta_{kk,is} \right\}.$$

This is the well known Kröner solution, presented in [18].

From (4.23) and (4.15) the following expression for the strain field due to a disclination follows:

$$(4.28) e_{is} = -K_{ij} + c_{jklm} \nabla_k \nabla_a \varepsilon_{smp} \varepsilon_{alb} [\varepsilon_{brn} \nabla_r \alpha_{np} + \theta_{bp} - \varepsilon_{pbr} \nabla_r \mathring{\varkappa}_{aa}]_{\langle is \rangle}$$

$$= -K_{ij} + c_{jklm} \nabla_k \nabla_a \varepsilon_{smp} [\nabla_a \alpha_{lp} - \nabla_l \alpha_{ap} + \varepsilon_{alb} \theta_{bp}]$$

$$+ K_{ij} + c_{jklm} \nabla_k \nabla_a [\varepsilon_{als} \nabla_m \mathring{\varkappa}_{aa} - \varepsilon_{alm} \nabla_s \mathring{\varkappa}_{aa}]_{\langle is \rangle}$$

$$= G_{ij} + c_{jklm} \nabla_k \varepsilon_{smp} \alpha_{lp} + K_{ij} + c_{jklm} \nabla_k \nabla_a \varepsilon_{smp} \varepsilon_{lab} \theta_{bp}$$

$$- \varepsilon_{isa} \nabla_a \mathring{\varkappa}_{aa} + \frac{1}{4\pi r} + \varepsilon_{isp} \nabla_a \alpha_{ap} + \frac{1}{4\pi r} \langle is \rangle,$$

$$(4.29) e_{is} = G_{ij} + C_{jklm} \nabla_k \varepsilon_{smp} \alpha_{lp} + K_{ij} + C_{jklm} \nabla_k \nabla_a \varepsilon_{smp} \varepsilon_{alb} \theta_{bp \langle is \rangle}.$$

If for the rectilinear disclination its line L coincides with the rotation axis, $\alpha = 0$, and e depends on θ only.

5. Conclusions

We have demonstrated the transitions from the theory of surface defects in the displacement description to the theories making use of the ideas of elastic and plastic deformations and what is called the incompatibility problem. In every formulation the theory breaks up into the conditions referring the form of elastic deformation (we call them here the geometric conditions), which are the constraints equations for the elastic fields, and the conditions of elastic equilibrium, together with the method of evaluating the elastic fields

when the constraints are prescribed. Formal solutions of the equilibrium equations are constructed by means of the Green tensor of the medium with a given symmetry. The physical quantities—the appropriate elastic fields—we express by means of physical source functions, the densities of the appropriate defects. In the incompatibility problem, the source quantity is the incompatibility of the initial strain.

In the second part of this work, we shall discuss the dynamic problems of the medium with defects.

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